LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100788.D
Acq On : 21 Nov 2017 18:46
Operator : SJ/JU
Sample : I6499-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PG1-2-E(4-5)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.104 | 509 | 513 | 523 | rVB | 81611 | 104215 | 5.61% | 0.683% |
| 2 | 5.493 | 574 | 579 | 582 | rBV | 1605018 | 1493120 | 80.40% | 9.782% |
| 3 | 6.498 | 745 | 750 | 755 | rBV | 1476501 | 1572806 | 84.70% | 10.304% |
| 4 | 6.640 | 770 | 774 | 778 | rBV | 1667033 | 1559335 | 83.97% | 10.216% |
| 5 | 6.869 | 810 | 813 | 817 | rBV | 533687 | 478060 | 25.74% | 3.132% |
| 6 | 7.028 | 836 | 840 | 843 | rBV | 1505952 | 1243668 | 66.97% | 8.148% |
| 7 | 7.434 | 904 | 909 | 912 | rBV | 1054609 | 950368 | 51.18% | 6.226% |
| 8 | 8.151 | 1027 | 1031 | 1035 | rBV | 756474 | 628679 | 33.85% | 4.119% |
| 9 | 9.228 | 1209 | 1214 | 1217 | rBV | 2188773 | 1857017 | 100.00% | 12.166% |
| 10 | 9.304 | 1223 | 1227 | 1229 | rBV | 25367 | 22351 | 1.20% | 0.146% |
| 11 | 9.616 | 1277 | 1280 | 1283 | rBV | 165701 | 140348 | 7.56% | 0.919% |
| 12 | 9.833 | 1313 | 1317 | 1320 | rVB | 60651 | 50982 | 2.75% | 0.334% |
| 13 | 9.910 | 1326 | 1330 | 1333 | rBV | 781228 | 667205 | 35.93% | 4.371% |
| 14 | 10.327 | 1399 | 1401 | 1404 | rVB | 66625 | 51835 | 2.79% | 0.340% |
| 15 | 10.551 | 1434 | 1439 | 1441 | rBV | 19278 | 23060 | 1.24% | 0.151% |
| 16 | 10.698 | 1460 | 1464 | 1467 | rBV | 901753 | 851429 | 45.85% | 5.578% |
| 17 | 10.804 | 1478 | 1482 | 1487 | rBV | 60956 | 61322 | 3.30% | 0.402% |
| 18 | 11.251 | 1554 | 1558 | 1560 | rBV | 43028 | 32716 | 1.76% | 0.214% |
| 19 | 11.392 | 1579 | 1582 | 1585 | rBV | 665575 | 610104 | 32.85% | 3.997% |
| 20 | 11.416 | 1585 | 1586 | 1590 | rVB | 65819 | 42633 | 2.30% | 0.279% |
| 21 | 11.910 | 1665 | 1670 | 1677 | rBV2 | 52703 | 51514 | 2.77% | 0.337% |
| 22 | 12.604 | 1785 | 1788 | 1792 | rBV | 71695 | 58134 | 3.13% | 0.381% |
| 23 | 12.833 | 1822 | 1827 | 1831 | rBV | 59955 | 63281 | 3.41% | 0.415% |
| 24 | 12.974 | 1847 | 1851 | 1855 | rBV | 1338521 | 1279098 | 68.88% | 8.380% |
| 25 | 13.863 | 1998 | 2002 | 2011 | rVB2 | 129946 | 145335 | 7.83% | 0.952% |
| 26 | 14.033 | 2027 | 2031 | 2034 | rBV | 530579 | 484358 | 26.08% | 3.173% |
| 27 | 14.192 | 2051 | 2058 | 2063 | rBV7 | 10741 | 26655 | 1.44% | 0.175% |
| 28 | 14.498 | 2106 | 2110 | 2112 | rBV3 | 18081 | 26606 | 1.43% | 0.174% |
| 29 | 15.068 | 2203 | 2207 | 2210 | rBV | 27545 | 39079 | 2.10% | 0.256% |
| 30 | 15.374 | 2256 | 2259 | 2266 | rVB2 | 17972 | 24402 | 1.31% | 0.160% |
| 31 | 15.439 | 2266 | 2270 | 2275 | rBV | 25593 | 33717 | 1.82% | 0.221% |
| 32 | 15.504 | 2276 | 2281 | 2289 | rBV | 399181 | 536864 | 28.91% | 3.517% |
| 33 | 16.004 | 2362 | 2366 | 2374 | rBV7 | 13015 | 25994 | 1.40% | 0.170% |
| 34 | 16.980 | 2527 | 2532 | 2536 | rBV2 | 14341 | 27583 | 1.49% | 0.181% |

LSC Area Percent Report

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Data File : BF100788.D
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Operator : SJ/JU
Sample : I6499-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PG1-2-E(4-5)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 15263873

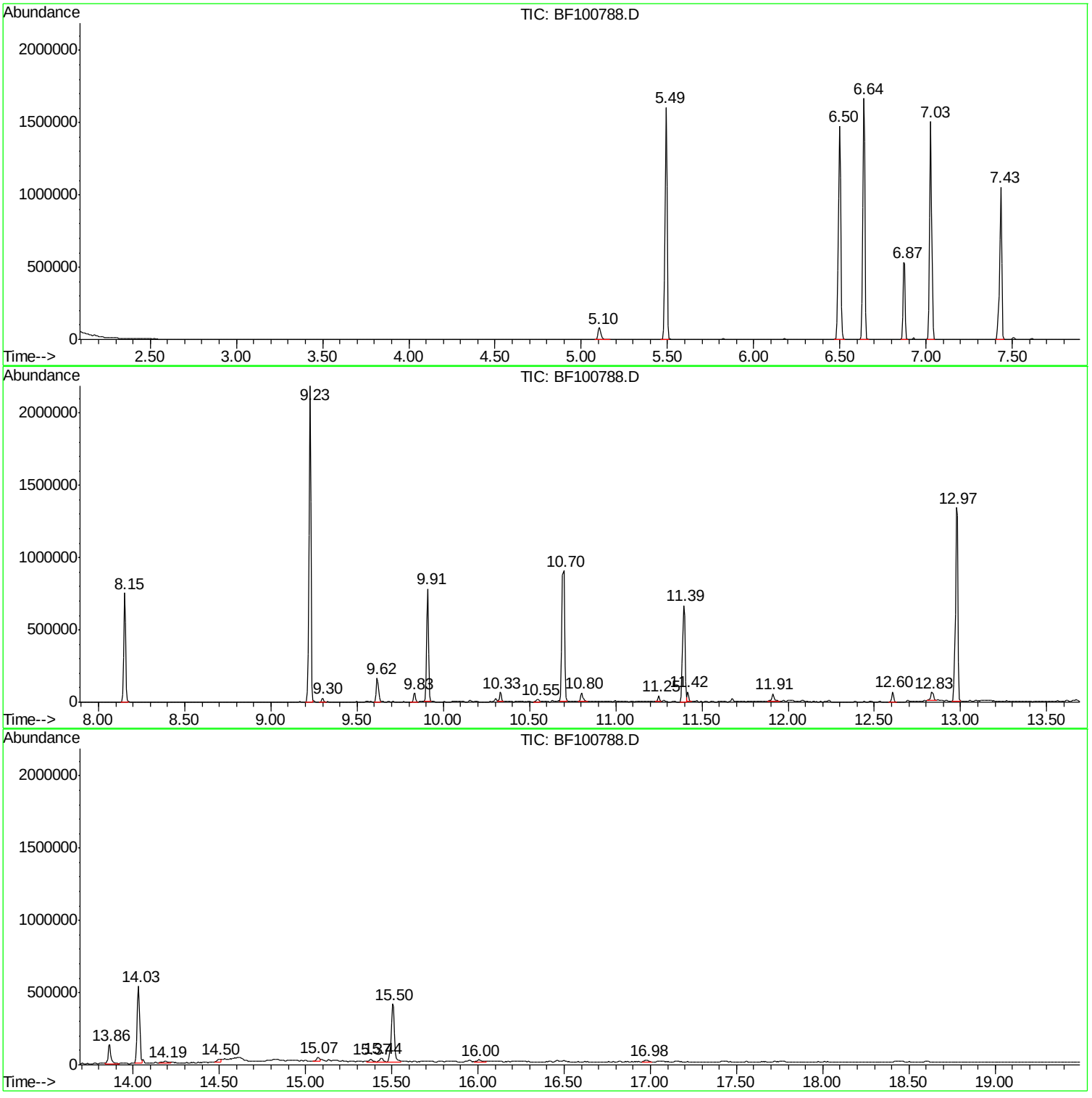
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100788.D
Acq On : 21 Nov 2017 18:46
Operator : SJ/JU
Sample : I6499-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PG1-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100788.D
Acq On : 21 Nov 2017 18:46
Operator : SJ/JU
Sample : I6499-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PG1-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

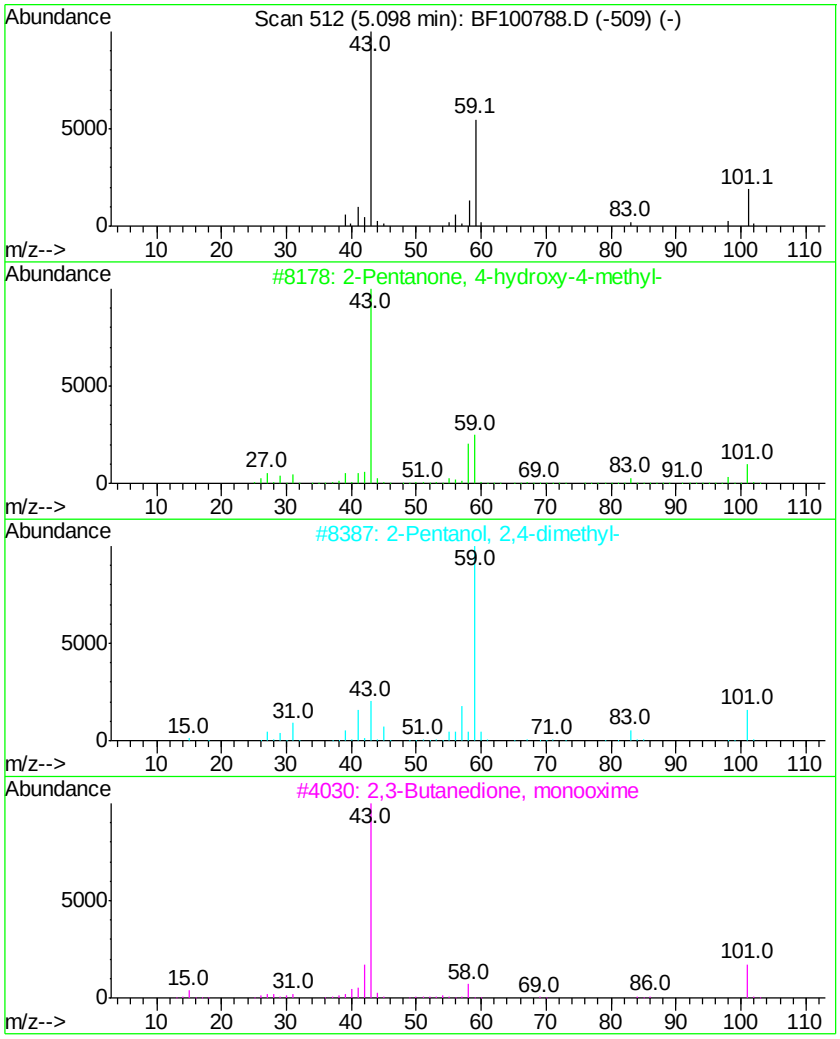
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

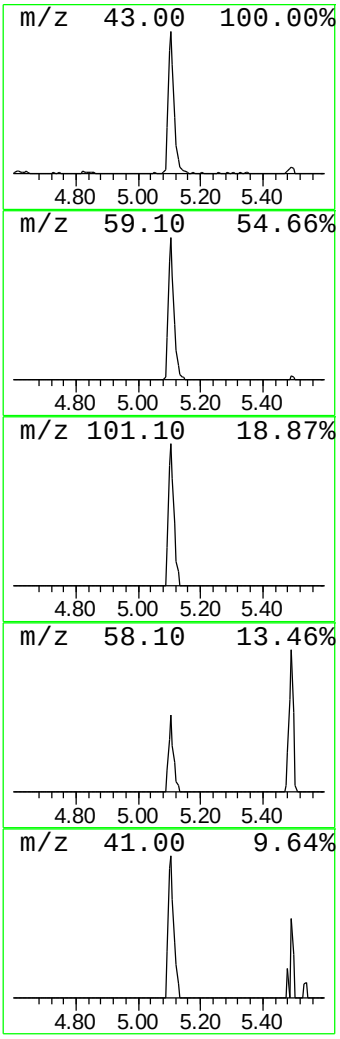
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.10 | 4.36 ng | 104215 | 1,4-Dichlorobenzene-d4 | 6.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | 2-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000625-06-9 | 25 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 4 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 5 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100788.D
Acq On : 21 Nov 2017 18:46
Operator : SJ/JU
Sample : I6499-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PG1-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

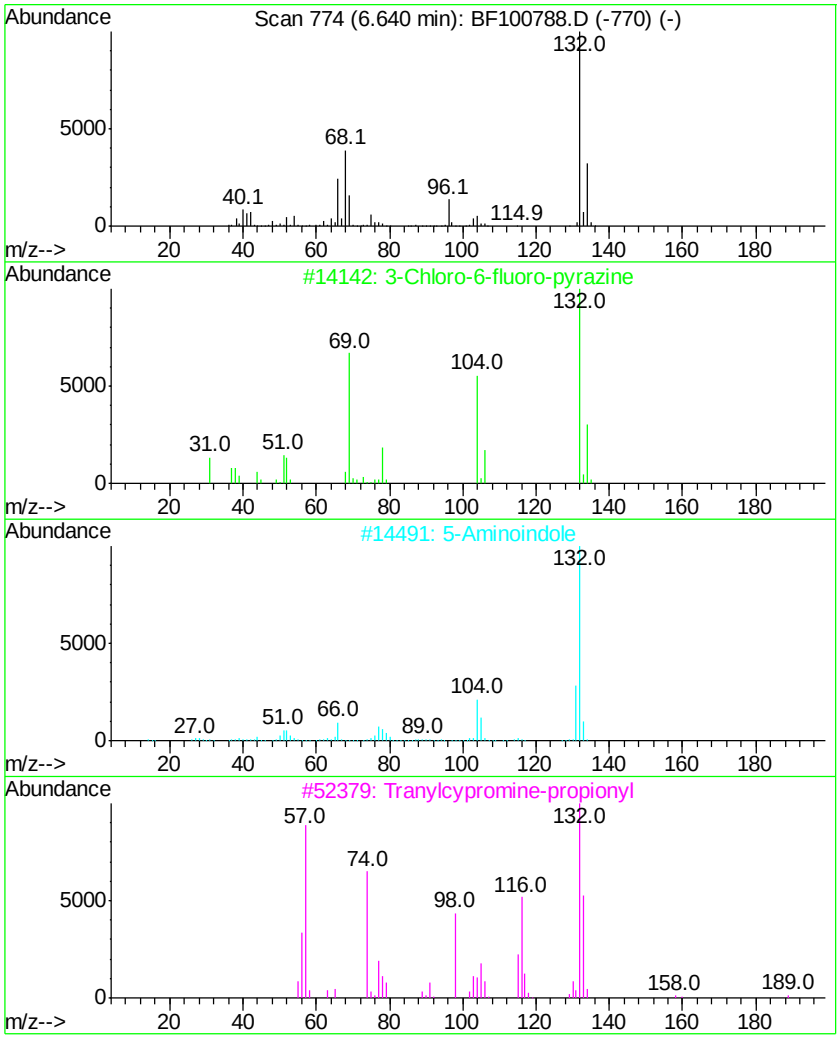
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

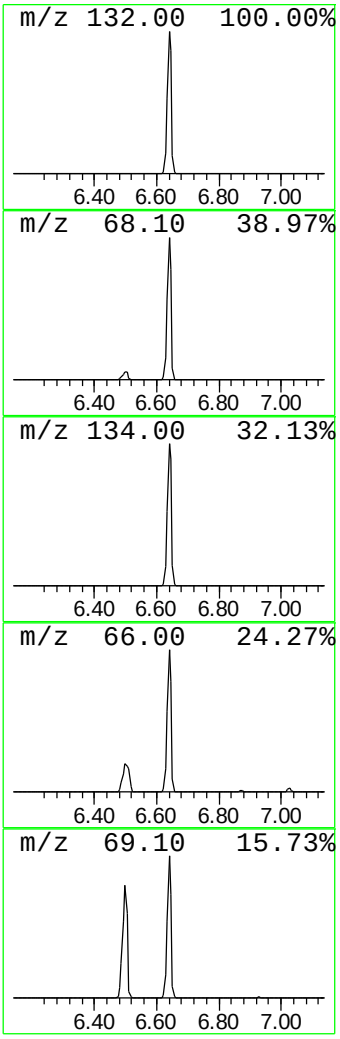
**********

Peak Number 2 unknown6.64 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.64 | 65.24 ng | 1559340 | 1,4-Dichlorobenzene-d4 | 6.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 9 |
| 5 | 4-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-60-2 | 9 |



# Library Search Compound Report

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Operator : SJ/JU
Sample : I6499-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PG1-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

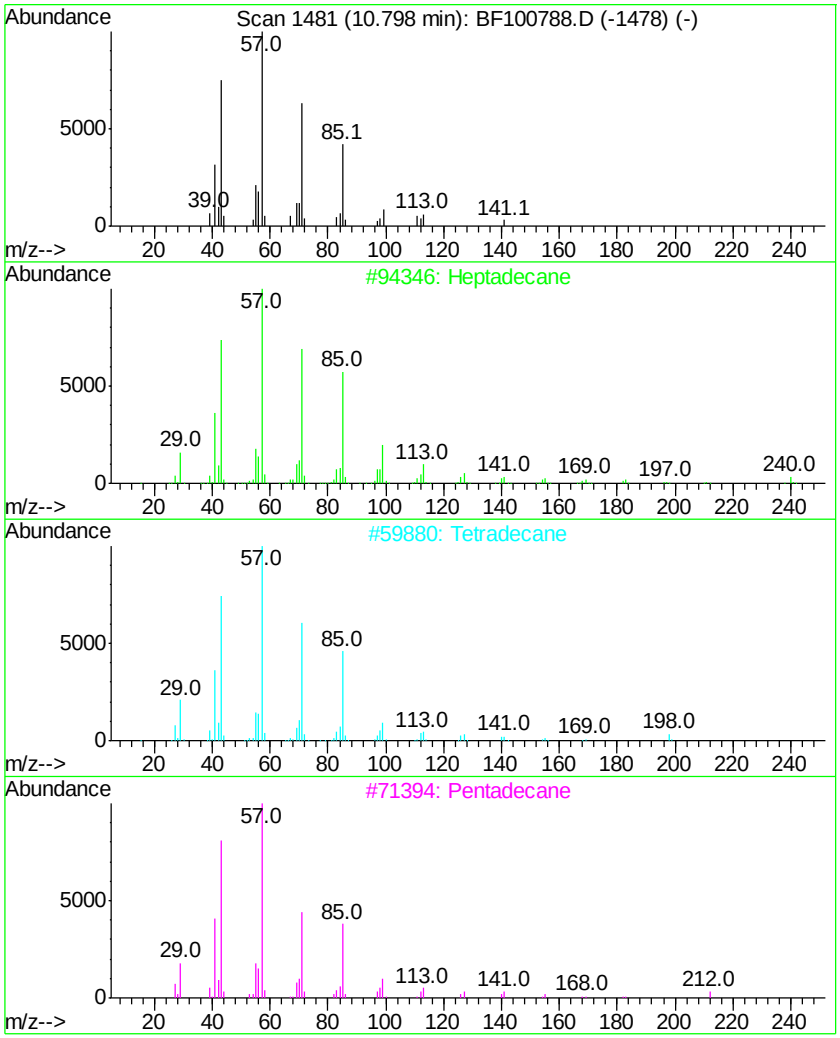
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

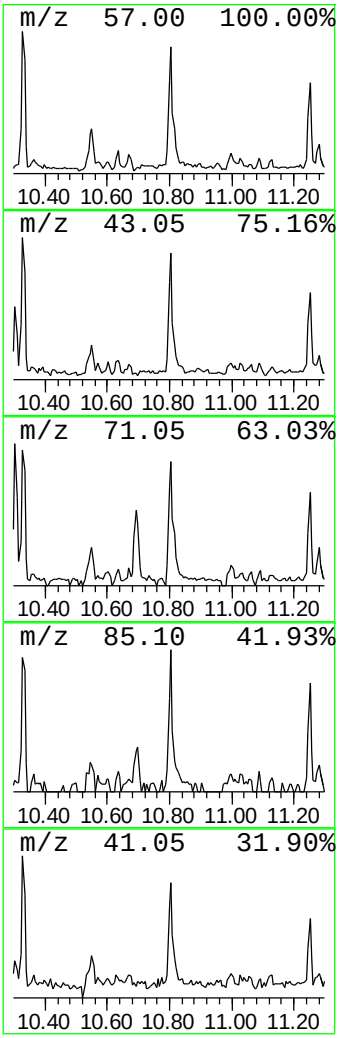
**********

Peak Number 4 Heptadecane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.80 | 2.01 ng | 61322 | Phenanthrene-d10 | 11.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 87 |
| 2 | Tetradecane | 198 | C14H30 | 000629-59-4 | 86 |
| 3 | Pentadecane | 212 | C15H32 | 000629-62-9 | 86 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 78 |
| 5 | Heptacosane | 380 | C27H56 | 000593-49-7 | 64 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100788.D
Acq On : 21 Nov 2017 18:46
Operator : SJ/JU
Sample : I6499-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PG1-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

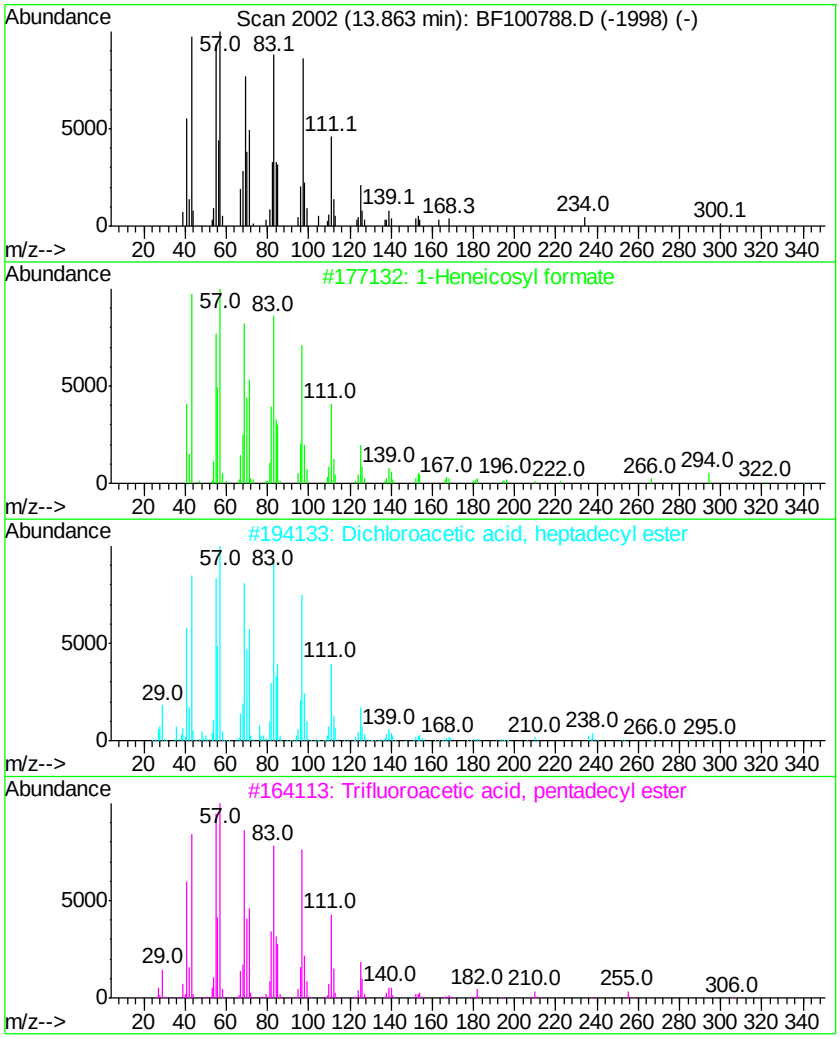
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

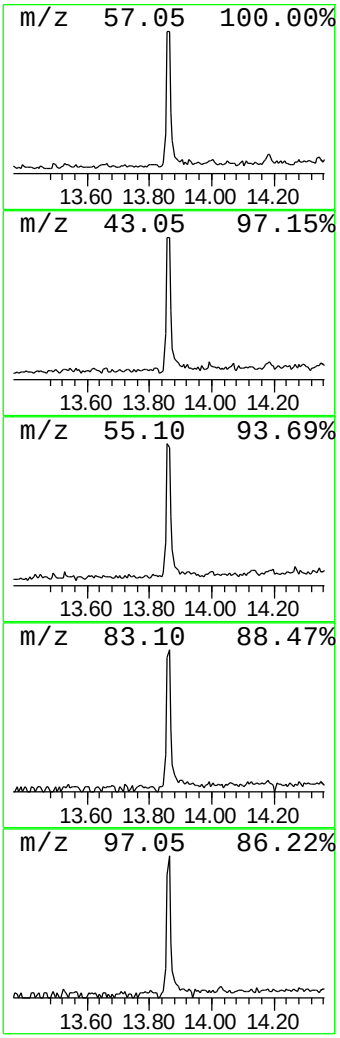
**********

Peak Number 6 1-Heneicosyl formate Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.86 | 6.00 ng | 145335 | Chrysene-d12 | 14.03 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosyl formate | 340 | C22H44O2 | 077899-03-7 | 95 |
| 2 | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 95 |
| 3 | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 94 |
| 4 | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 94 |
| 5 | Heptafluorobutyric acid, n-tetra... | 410 | C18H29F7O2 | 007365-36-8 | 94 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112117\
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Misc :
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**Instrument :** BNA_F
**ClientSampleId :** PG1-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 5.10 | 4.4 | ng | 104215 | 1 | 6.87 | 478060 | 20.0 |
| unknown6.64 | 6.64 | 65.2 | ng | 1559340 | 1 | 6.87 | 478060 | 20.0 |
| Heptadecane | 10.80 | 2.0 | ng | 61322 | 4 | 11.39 | 610104 | 20.0 |
| 1-Heneicosyl formate | 13.86 | 6.0 | ng | 145335 | 5 | 14.03 | 484358 | 20.0 |